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14. ABSTRACT

A supercritical hydrocarbon impinging injector simulation facility was procured and installed to increase the available computational capability to conduct molecular dynamics simulations of supercritical impinging injectors using hydrocarbon propellants. Supercritical impinging injectors using hydrocarbon propellants are of interest to the next generation of liquid propellant rocket engines. The procured high performance computing cluster allows simulations to be conducted in a sufficiently short time period to allow investigation of the effects of operating conditions, injector geometry and propellant composition on the propellant mixing process. Such a facility provides valuable information on the operating characteristics of supercritical hydrocarbon impinging injectors as well as increases the exposure of graduate and undergraduate students to the use of parallel computers to solve engineering and scientific problems of interest to the Air Force. Initial impinging injector simulations have reproduced the differing behavior between subcritical and supercritical liquid nitrogen injection behavior, including the disappearance of surface tension above the propellant critical point. The use of molecular dynamics to simulate the mixing process eliminates the need to track phase boundaries under subcritical conditions, and automatically incorporates rapidly varying material properties near the critical point and mixture effects. Current algorithm development involves the simulation of the ethanol and heptane.

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Supercritical Hydrocarbon Impinging Injector Simulation Facility

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Abstract

A supercritical hydrocarbon impinging injector simulation facility was procured and installed to increase the available computational capability to conduct molecular dynamics simulations of supercritical impinging injectors using hydrocarbon propellants. Supercritical impinging injectors using hydrocarbon propellants are of interest to the next generation of liquid propellant rocket engines. The procured high performance computing cluster allows simulations to be conducted in a sufficiently short time period to allow investigation of the effects of operating conditions, injector geometry and propellant composition on the propellant mixing process. Such a facility provides valuable information on the operating characteristics of supercritical hydrocarbon impinging injectors as well as increases the exposure of graduate and undergraduate students to the use of parallel computers to solve engineering and scientific problems of interest to the Air Force. Initial impinging injector simulations have reproduced the differing behavior between subcritical and supercritical liquid nitrogen injection behavior, including the disappearance of surface tension above the propellant critical point. The use of molecular dynamics to simulate the mixing process eliminates the need to track phase boundaries under subcritical conditions, and automatically incorporates rapidly varying material properties near the critical point and mixture effects. Current algorithm development involves the simulation of the ethanol and heptane.

Introduction

Research is currently being conducted under AFOSR Grant FA9550-04-1-0012 (Principal Investigator: Dr. Michael M. Micci) to investigate the transcritical and supercritical mixing of a liquid injected into a gaseous environment using molecular dynamics (MD). This program is being funded at the level of $54K/year under the management of Dr. Mitat Birkan. The problem has direct application to the next generation of liquid propellant rocket engines being designed for quick response Earth launch operations. The use of MD to simulate the mixing process eliminates the need to track phase boundaries under subcritical conditions, and automatically incorporates rapidly varying material properties near the critical point and mixture effects. Recent simulation results for radial density profiles for liquid nitrogen injection into supercritical gaseous nitrogen match experimental results obtained at DLR Lampoldshausen[1,2].

The MD computations are parallelized using MPI. The simulations are performed on a PC Beowulf cluster that was purchased under a previous AFOSR Grant (F49620-01-1-0432) managed by Dr. Mitat Birkan. The cluster consists of 22 Intel Pentium 1 GHz processors and 20 Intel Xeon 2.4 GHz processors connected by an Ethernet switch. The system is configured as two separate subclusters due to the processing speed difference between the two processor types, which were purchased two years apart. Thus the codes currently in use are parallelized to use 16 – 22 processors.

Interest also exists in the use of impinging injectors in liquid propellant rocket engines when both the fuel and the oxidizer enter the combustion chamber as liquids. The primary example of a propellant combination used with impinging injectors is a liquid hydrocarbon such as RP-1 as the fuel and liquid oxygen as the oxidizer. An example of the current state-of-the-art for impinging injectors is the platelet injector developed by the Aerojet Corporation, where typical orifice sizes are of the order of 127 microns[3].

Procured Facility

A Western Scientific Fusion A64 Solution Cluster was purchased and installed with the funding provided by this grant. The Cluster consists of 24 (1 head and 23 compute) nodes, where each node contains two Opteron 265 1.8 GHz dual core processors along with 4GB of memory and a 40GB hard drive. The nodes are connected by a Voltaire ISR9024 Infiniband Switch Router to give a faster communication speed than can be provided by high speed Ethernet without the cost of a Myrinet network. Redhat Linux is used as the operating system with Portland Group compilers for several versions of Fortran and C. The Cluster provides both a high computational speed with large on-board memory and fast communications between nodes when needed for a relatively low cost.

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[1] "Molecular Dynamics Simulation of Supercritical Hydrocarbons," R. D. Branam, K. F. Ludwig and M. M. Micci. Proceedings of the 17th Annual Conference on Liquid Atomization and Spray Systems, Arlington, VA, May 17-19, 2004.

[2] "Molecular Dynamics Simulations of Supercritical Jet Mixing," M. M. Micci, R. D. Branam and K. F. Ludwig. Proceedings of the International Symposium on Energy Conversion Fundamentals, Istanbul, Turkey, June 21-25, 2004.

[3] "Platelet Injectors for Space Shuttle Orbit Maneuvering Engine," R. C. Kahl, R. J. Labotz and L. B. Bassham, AIAA Paper 1974-1108.

Results to Date

In order to investigate the mixing process for impinging injection under subcritical and supercritical combustion chamber conditions, an MD simulation of impinging liquid nitrogen injection was initially developed. The impinging injection simulation is a modification of the single liquid injection simulation previously developed where a second liquid stream is computationally generated and the two streams are injected at an angle toward each other. Figure 1 shows the MD result at the beginning of a simulation where the blue and green indicate nitrogen molecules in the two liquid streams and the red molecules indicate the gaseous nitrogen.

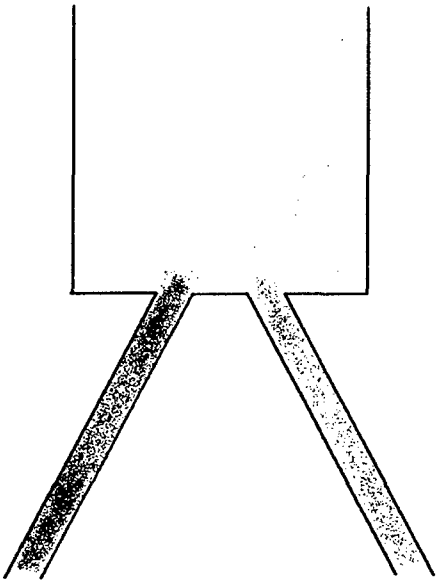

Fig. 1 Initial configuration for the MD simulation of impinging liquid nitrogen injection. The blue and green indicate nitrogen molecules in the two liquid streams and the red molecules are the gaseous nitrogen

Impinging injection simulations were carried out using liquid nitrogen as the injected liquid under both subcritical and supercritical conditions. The subcritical conditions were 94 K and 0.5 MPa while the supercritical conditions were at 300 K and 4 MPa. The critical temperature and pressure for nitrogen is 126 K and 3.38 MPa respectively. Significant differences between the subcritical and the supercritical simulations in the morphology of the mixing between the two liquids streams are evident. Figure 2 shows density contours in the plane containing the two injectors for the injection of two liquid nitrogen streams into subcritical nitrogen gas. It can be seen that, as expected under subcritical conditions, the two liquid streams are beginning to merge to form a fan shaped liquid sheet prior to primary and then secondary atomization. The effect of surface tension causing the formation of a droplet is visible. Although Figure 2 shows the last computed time, the injection is still transient and the steady state has yet to be reached. Temperature contours are also computed and for the subcritical case show the same morphology as the density contours.

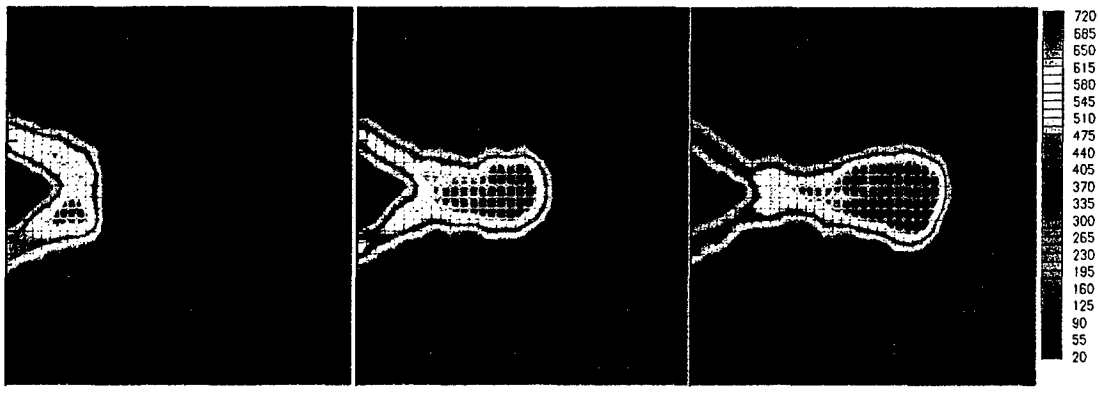

Fig. 2 Density contours in the plane containing two impinging injectors for liquid nitrogen under subcritical conditions (94 K, 0.5 MPa).

Under supercritical conditions a radically different mixing pattern develops. Figure 3 shows a series of three density contours for two liquid nitrogen streams injected into a supercritical nitrogen environment. The surface tension of the injected liquid quickly disappears and the density contours show a greater asymmetry and disruption than the subcritical simulation. The absence of surface tension resulting in a gas-like mixing of the two streams is now seen along with the three-dimensional morphology of the process. Once again, even though the simulation was ended at the point shown in Figure 3, the mixing is still transient.

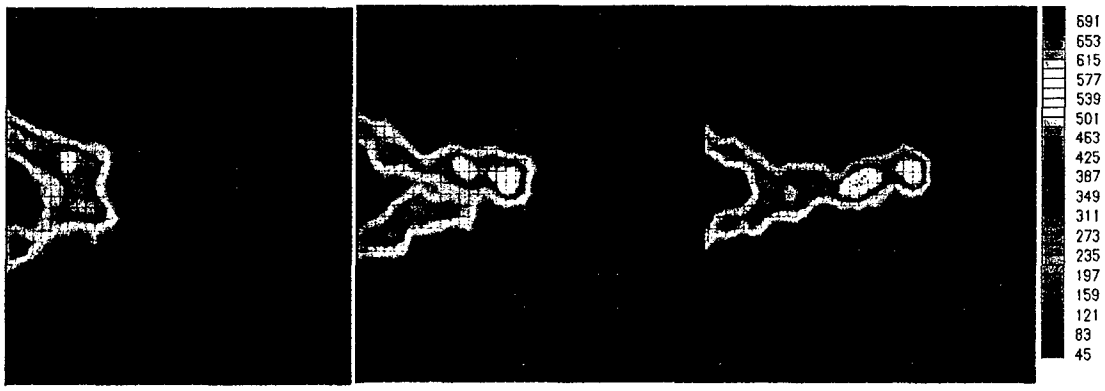

Fig. 3 Density contours in the plane containing two impinging injectors under supercritical chamber conditions (300 K and 4 MPa) showing absence of surface tension and gas-like mixing.

Liquid nitrogen is a convenient fluid to use to examine transcritical and supercritical mixing, both experimentally and computationally, and is a good simulant for liquid oxygen. But the behavior of liquid hydrocarbon mixtures used in impinging injectors under supercritical combustion chamber conditions is of primary interest to the design and development of the next generation of Earth launch engines. Thus the simulation of impinging injection using a hydrocarbon mixture representative of a typical liquid hydrocarbon fuel such as RP-1 was initiated this year. Hydrocarbons can be easily simulated using MD, however the computational cost increases due to the need to model separately each methyl or methylene interatomic

potential site in the molecule. While liquid nitrogen requires the computation of interatomic forces to and from two atomic nitrogen sites in each molecule, heptane would require the computation for seven sites and decane would require the computation for ten sites.

Heptane was selected as the initial hydrocarbon to model. In molecular dynamics simulations heptane is modeled as a CH_3 site on each end on the molecule and five CH_2 sites in between, each site being modeled as a separate Lennard-Jones 12-6 interatomic potential for a total of seven sites. Bond lengths and angles are fixed but a torsional potential is included, with all interatomic potential and structure parameters obtainable from the chemical literature[4,5]. The standard molecular dynamics algorithm RATTLE is used to efficiently maintain the bond lengths and angles through an iterative technique[6]. Work has also been initiated to model the ethanol molecule, although the ethanol molecule includes a Coulomb potential that, because of the longer range of its interaction, requires a larger number of neighboring molecules to be included in the force computation, increasing the computational workload.

Enhancement to Research-Related Education

Parallel computing is becoming the standard for high performance computing, both in the Department of Aerospace Engineering at The Pennsylvania State University as well as the world at large. The Department offers a graduate level course in parallel computing, AERSP 597D, Parallel Processing, which teaches the use of parallel computers to solve engineering and scientific problems. The addition of the above proposed computer cluster has allowed a number of both graduate and undergraduate students to have the opportunity to obtain experience in the use of parallel computers to solve problems of interest to the Air Force.

There are no publications, interactions/transitions, new discoveries, inventions, patent disclosures or honors/awards associated with this grant to report.

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[4] "Dynamics of Alkane Chains Included in an Organic Matrix: Molecular Dynamics Simulation and Comparison with Neutron Scattering Experiment," N.-D. Morelon, G. R. Kneller, M. Ferrand, A. Grand, J. C. Smith and M. Bee, *Journal of Chemical Physics*, Vol. 109, 1998, pp. 2883-2894.

[5] "The Adsorption and Localization of Mixtures of C4-C7 Alkane Isomers in Zeolites by Computer Simulation," L. Lu, Q. Wang and Y. Liu, *Journal of Physical Chemistry*, 2005.

[6] "Rattle: a 'Velocity' Version of the Shake Algorithm for Molecular Dynamics Calculations," H. C. Andersen, *Journal of Computational Physics*, Vol. 52, 1983, pp. 24-34.